



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:02 AM UTC

PDB ID : 6Z99 / pdb_00006z99
Title : Copper transporter OprC
Authors : Bhamidimarri, S.P.; van den Berg, B.
Deposited on : 2020-06-03
Resolution : 2.68 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

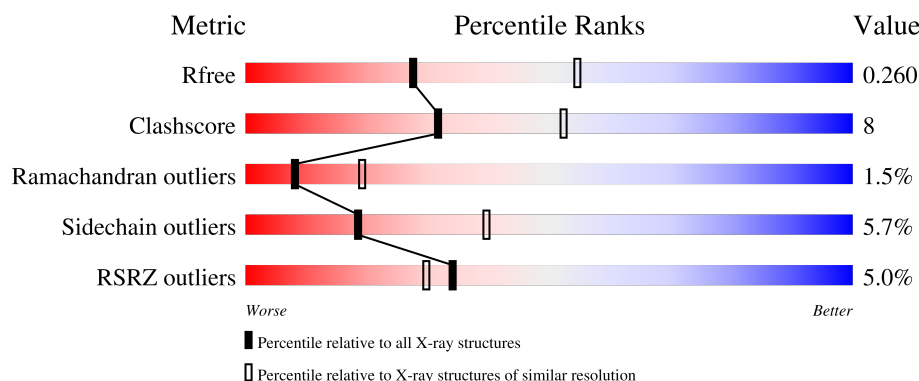
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	723	2% 74% 15% 10%
1	B	723	7% 69% 20% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AG	A	802	-	-	X	-
2	AG	B	803	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10196 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Putative copper transport outer membrane porin OprC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	654	Total	C	N	O	S	4	1	0
			5074	3185	896	977	16			
1	B	658	Total	C	N	O	S	4	2	0
			5108	3207	902	981	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	ALA	CYS	engineered mutation	UNP G3XD89
B	143	ALA	CYS	engineered mutation	UNP G3XD89

- Molecule 2 is SILVER ION (CCD ID: AG) (formula: Ag).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Ag	0	0
			3	3		
2	B	3	Total	Ag	0	0
			3	3		

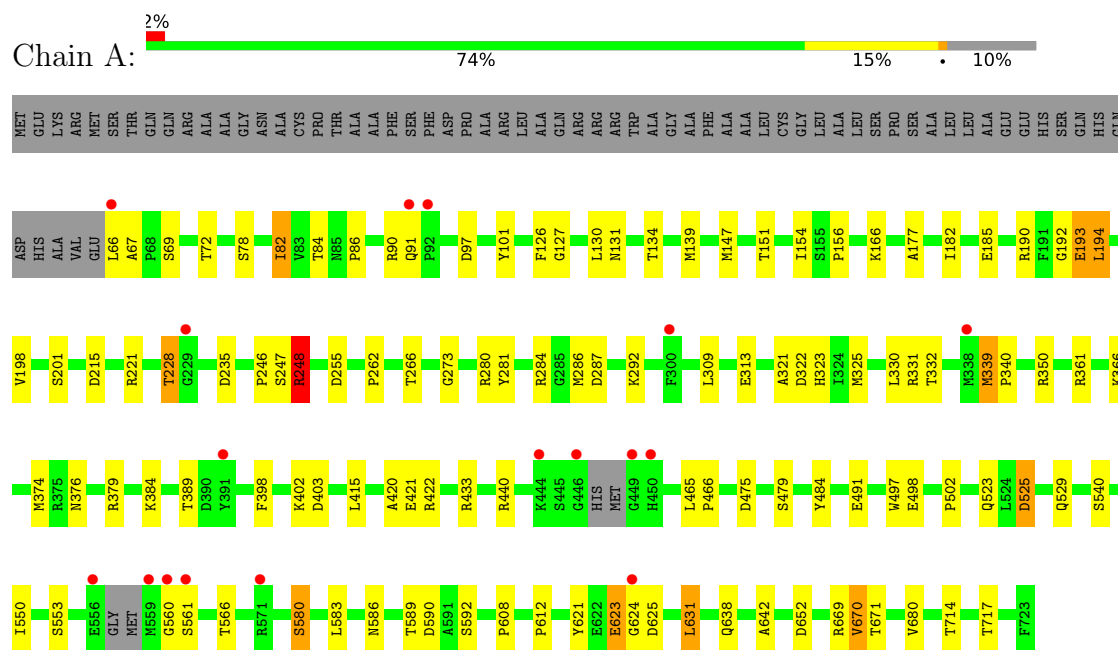
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		
3	B	2	Total	O	0	0
			2	2		

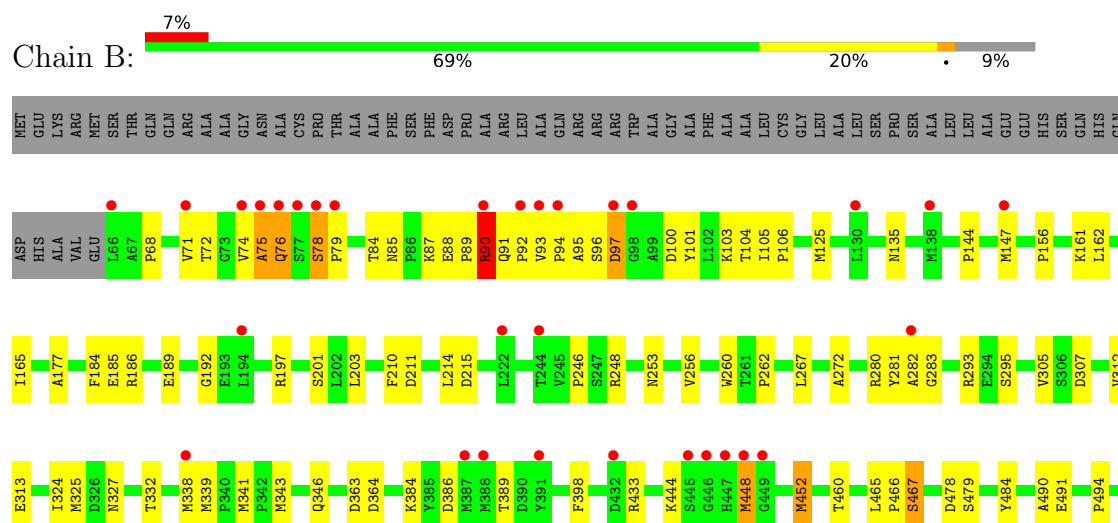
3 Residue-property plots

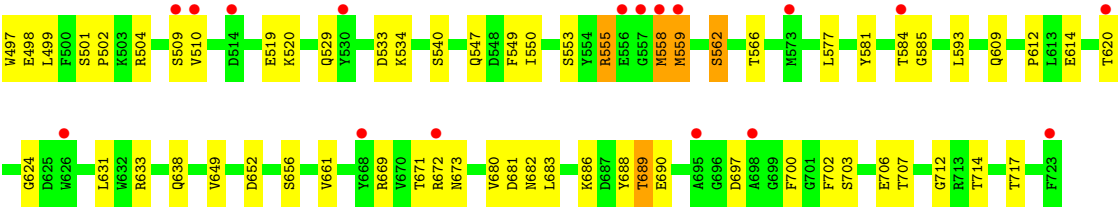
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Putative copper transport outer membrane porin OprC



- Molecule 1: Putative copper transport outer membrane porin OprC





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	154.64Å 195.51Å 165.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.18 – 2.68 84.18 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.8 (84.18-2.68) 99.9 (84.18-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.18_3855	Depositor
R, R_{free}	0.215 , 0.252 0.224 , 0.260	Depositor DCC
R_{free} test set	3459 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	67.0	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10196	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/5202	0.65	0/7051
1	B	0.39	0/5242	0.63	0/7107
All	All	0.40	0/10444	0.64	0/14158

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5074	0	4854	62	0
1	B	5108	0	4893	101	0
2	A	3	0	0	3	0
2	B	3	0	0	3	0
3	A	6	0	0	0	0
3	B	2	0	0	0	0
All	All	10196	0	9747	161	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (161) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:MET:HE1	2:B:803:AG:AG	1.55	0.92
1:B:72:THR:HA	1:B:92:PRO:HG3	1.52	0.92
1:A:286:MET:HE3	2:A:802:AG:AG	1.62	0.85
1:A:286:MET:CE	2:A:802:AG:AG	2.12	0.84
1:B:90:ARG:HH11	1:B:101:TYR:HB3	1.41	0.82
1:B:343:MET:CE	2:B:803:AG:AG	2.14	0.82
1:B:467:SER:HB3	1:B:490:ALA:HA	1.64	0.79
1:B:246:PRO:HG2	1:B:282:ALA:HB2	1.68	0.76
1:B:498:GLU:HG2	1:B:550:ILE:HG21	1.66	0.76
1:B:71:VAL:HB	1:B:90:ARG:HA	1.70	0.71
1:B:612:PRO:HB3	1:B:638:GLN:HB2	1.72	0.71
1:A:72:THR:HB	1:A:631:LEU:HD13	1.73	0.70
1:B:614:GLU:OE1	1:B:633:ARG:NE	2.24	0.69
1:A:147:MET:HE2	1:A:284:ARG:HD2	1.73	0.68
1:B:78:SER:HB3	1:B:79:PRO:CD	2.23	0.68
1:B:90:ARG:HE	1:B:101:TYR:HD2	1.42	0.67
1:B:246:PRO:HG3	1:B:700:PHE:CD1	2.29	0.67
1:B:94:PRO:HD3	1:B:681:ASP:OD2	1.96	0.65
1:B:484:TYR:HH	1:B:540:SER:HG	1.43	0.65
1:B:147:MET:HG2	1:B:281:TYR:CE2	2.32	0.65
1:B:84:THR:HG21	1:B:90:ARG:NH2	2.12	0.65
1:A:612:PRO:HB3	1:A:638:GLN:HB2	1.80	0.64
1:B:680:VAL:HG11	1:B:683:LEU:HD13	1.80	0.63
1:A:255:ASP:OD2	1:A:273:GLY:HA3	1.99	0.63
1:B:91:GLN:NE2	1:B:94:PRO:HA	2.14	0.63
1:A:498:GLU:HG2	1:A:550:ILE:HG21	1.81	0.62
1:B:682:ASN:HD21	1:B:686:LYS:H	1.48	0.62
1:A:580:SER:HB2	1:A:590:ASP:HB3	1.83	0.61
1:B:135:ASN:HD21	1:B:186:ARG:HB2	1.65	0.61
1:B:74:VAL:HB	1:B:105:ILE:HG12	1.82	0.61
1:B:91:GLN:HE22	1:B:94:PRO:HA	1.66	0.61
1:A:466:PRO:O	1:A:491:GLU:HG3	2.01	0.60
1:A:422:ARG:HB3	1:A:475:ASP:HB2	1.82	0.60
1:B:214:LEU:HD12	1:B:215:ASP:H	1.66	0.60
1:B:84:THR:HG22	1:B:162:LEU:HB3	1.82	0.60
1:B:491:GLU:CD	1:B:520:LYS:HD3	2.27	0.60
1:B:689:THR:HG21	1:B:707:THR:OG1	2.02	0.60
1:A:151:THR:HA	1:A:154:ILE:HD12	1.84	0.60
1:B:248:ARG:HH21	1:B:280:ARG:NH1	1.98	0.59
1:A:286:MET:HE2	2:A:802:AG:AG	1.89	0.58
1:A:466:PRO:HG2	1:B:466:PRO:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:GLN:NE2	1:B:652:ASP:OD1	2.37	0.58
1:A:583:LEU:HD11	1:A:589:THR:HG22	1.86	0.57
1:A:287:ASP:CG	1:A:331:ARG:HH21	2.12	0.57
1:A:484:TYR:OH	1:A:540:SER:HB3	2.04	0.57
1:B:90:ARG:NH1	1:B:101:TYR:O	2.38	0.56
1:B:72:THR:HB	1:B:631:LEU:HD13	1.88	0.56
1:B:497:TRP:O	1:B:502:PRO:HD3	2.06	0.56
1:A:72:THR:HG22	1:A:91:GLN:HB3	1.88	0.56
1:B:253:ASN:HD22	1:B:293:ARG:HH21	1.53	0.56
1:A:379:ARG:HG2	1:A:402:LYS:HA	1.88	0.55
1:A:608:PRO:HB3	1:A:642:ALA:HB3	1.88	0.55
1:B:248:ARG:HH21	1:B:280:ARG:HH12	1.55	0.54
1:B:74:VAL:HG21	1:B:90:ARG:NH2	2.22	0.54
1:B:84:THR:HG21	1:B:90:ARG:HH22	1.72	0.54
1:B:534:LYS:HB2	1:B:581:TYR:HE2	1.71	0.54
1:A:193:GLU:HG3	1:A:194:LEU:N	2.24	0.53
1:B:91:GLN:CD	1:B:94:PRO:HA	2.34	0.53
1:A:262:PRO:HD2	1:A:266:THR:HB	1.90	0.53
1:B:497:TRP:O	1:B:501:SER:HB2	2.09	0.52
1:B:91:GLN:OE1	1:B:94:PRO:HA	2.09	0.52
1:B:384:LYS:HG3	1:B:398:PHE:CZ	2.45	0.52
1:B:386:ASP:HB3	1:B:389:THR:HG22	1.92	0.52
1:B:93:VAL:HA	1:B:681:ASP:OD2	2.10	0.51
1:B:260:TRP:NE1	1:B:262:PRO:HG3	2.26	0.51
1:B:324:ILE:HG13	1:B:346:GLN:HG3	1.90	0.51
1:A:280:ARG:HG3	1:A:330:LEU:HB3	1.93	0.51
1:B:327:ASN:ND2	1:B:339:MET:HE2	2.25	0.51
1:B:91:GLN:HE22	1:B:94:PRO:CA	2.23	0.50
1:B:363:ASP:OD2	1:B:364:ASP:N	2.44	0.50
1:B:78:SER:HB3	1:B:79:PRO:HD2	1.93	0.50
1:B:92:PRO:HG2	1:B:104:THR:HG22	1.92	0.50
1:B:702:PHE:HD1	1:B:706:GLU:HG2	1.76	0.50
1:A:669:ARG:HG3	1:A:669:ARG:HH11	1.77	0.49
1:B:203:LEU:O	1:B:210:PHE:HA	2.13	0.49
1:A:523:GLN:NE2	1:A:525:ASP:OD2	2.38	0.49
1:B:555:ARG:NE	1:B:555:ARG:HA	2.27	0.49
1:B:577:LEU:HD21	1:B:593:LEU:HD23	1.94	0.49
1:A:465:LEU:HB3	1:A:491:GLU:HB2	1.95	0.48
1:A:287:ASP:OD2	1:A:331:ARG:NE	2.31	0.48
1:A:497:TRP:O	1:A:502:PRO:HD3	2.12	0.48
1:B:448:MET:HE3	1:B:559:MET:HE2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ARG:HD2	1:A:366:LYS:HB2	1.96	0.48
1:A:339:MET:H	1:A:340:PRO:HD3	1.79	0.48
1:A:384:LYS:HD2	1:A:398:PHE:CZ	2.49	0.48
1:A:84:THR:HG21	1:A:90:ARG:HH22	1.79	0.48
1:A:130:LEU:HD23	1:A:182:ILE:CD1	2.44	0.48
1:B:75:ALA:HA	1:B:106:PRO:CD	2.44	0.48
1:A:190:ARG:HB3	1:A:190:ARG:NH1	2.29	0.47
1:A:403:ASP:HB2	1:A:440:ARG:CG	2.44	0.47
1:B:555:ARG:HA	1:B:555:ARG:HE	1.79	0.47
1:A:350:ARG:O	1:A:376:ASN:HA	2.14	0.47
1:B:478:ASP:N	1:B:478:ASP:OD1	2.43	0.47
1:B:534:LYS:HB2	1:B:581:TYR:CE2	2.50	0.47
1:A:86:PRO:HA	1:A:90:ARG:NH1	2.30	0.46
1:A:323:HIS:NE2	1:A:325:MET:HG3	2.30	0.46
1:A:139:MET:CE	1:A:321:ALA:HB2	2.44	0.46
1:A:101:TYR:CD1	1:A:156:PRO:HG2	2.51	0.46
1:A:235:ASP:HA	1:A:248:ARG:HB2	1.97	0.46
1:B:95:ALA:HA	1:B:100:ASP:HB3	1.98	0.46
1:B:144:PRO:O	1:B:497:TRP:HD1	1.98	0.46
1:B:68:PRO:HG3	1:B:669:ARG:HB2	1.97	0.46
1:A:192:GLY:O	1:A:221:ARG:HG3	2.16	0.46
1:B:577:LEU:CD2	1:B:593:LEU:HB3	2.46	0.46
1:A:433:ARG:NH1	1:B:547:GLN:OE1	2.49	0.46
1:A:529:GLN:HE21	1:A:529:GLN:HB3	1.64	0.45
1:B:101:TYR:CD1	1:B:156:PRO:HG2	2.52	0.45
1:A:215:ASP:HB2	1:A:228:THR:HG22	1.97	0.45
1:A:374:MET:HE3	1:A:374:MET:HB3	1.77	0.45
1:B:125:MET:HA	1:B:125:MET:HE2	1.98	0.45
1:B:452:MET:HB3	1:B:452:MET:HE2	1.49	0.45
1:B:78:SER:HA	1:B:529:GLN:OE1	2.17	0.45
1:B:74:VAL:O	1:B:75:ALA:C	2.60	0.45
1:B:712:GLY:O	1:B:714:THR:HG23	2.17	0.45
1:B:661:VAL:HG21	1:B:688:TYR:CZ	2.52	0.44
1:A:72:THR:HG22	1:A:91:GLN:CB	2.47	0.44
1:B:72:THR:CA	1:B:92:PRO:HG3	2.35	0.44
1:B:519:GLU:HG3	1:B:549:PHE:HA	1.99	0.44
1:B:633:ARG:HH22	1:B:690:GLU:CD	2.26	0.44
1:A:147:MET:HB3	1:A:281:TYR:HE2	1.83	0.44
1:A:151:THR:HA	1:A:154:ILE:CD1	2.47	0.44
1:A:624:GLY:O	1:A:625:ASP:HB2	2.16	0.44
1:B:91:GLN:HE22	1:B:94:PRO:HB3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:MET:HE2	1:B:448:MET:HE1	2.00	0.44
1:B:144:PRO:HD2	1:B:325:MET:HE1	2.00	0.43
1:B:343:MET:HE2	2:B:803:AG:AG	1.98	0.43
1:B:433:ARG:HH11	1:B:433:ARG:HG2	1.83	0.43
1:B:702:PHE:CD1	1:B:706:GLU:HG2	2.52	0.43
1:B:162:LEU:HD13	1:B:184:PHE:CD1	2.54	0.43
1:B:88:GLU:O	1:B:90:ARG:N	2.51	0.43
1:B:189:GLU:OE1	1:B:197:ARG:NH2	2.51	0.43
1:B:283:GLY:HA2	1:B:697:ASP:N	2.34	0.43
1:A:623:GLU:HB3	1:A:624:GLY:H	1.53	0.43
1:B:671:THR:HG22	1:B:672:ARG:N	2.34	0.43
1:A:131:ASN:HB2	1:A:177:ALA:HB2	2.01	0.43
1:A:560:GLY:O	1:A:561:SER:OG	2.35	0.42
1:B:135:ASN:OD1	1:B:186:ARG:N	2.42	0.42
1:B:533:ASP:CG	1:B:534:LYS:H	2.27	0.42
1:B:100:ASP:HA	1:B:103:LYS:HE2	2.00	0.42
1:B:584:THR:HG22	1:B:585:GLY:N	2.34	0.42
1:A:583:LEU:CD1	1:A:589:THR:HG22	2.48	0.42
1:A:586:ASN:O	1:A:621:TYR:HA	2.20	0.42
1:A:670:VAL:HG23	1:A:671:THR:HG23	2.02	0.42
1:B:272:ALA:HA	1:B:295:SER:O	2.20	0.42
1:B:85:ASN:OD1	1:B:87:LYS:HB2	2.19	0.42
1:A:670:VAL:CG2	1:A:671:THR:HG23	2.50	0.42
1:B:74:VAL:O	1:B:74:VAL:HG12	2.20	0.41
1:B:74:VAL:HG11	1:B:84:THR:HB	2.01	0.41
1:B:161:LYS:HB3	1:B:185:GLU:HG3	2.02	0.41
1:A:82:ILE:HD11	1:A:166:LYS:HE2	2.03	0.41
1:A:669:ARG:HG3	1:A:669:ARG:NH1	2.36	0.41
1:B:494:PRO:HB2	1:B:499:LEU:HG	2.03	0.41
1:B:504:ARG:NH1	1:B:562:SER:OG	2.51	0.41
1:B:671:THR:HG22	1:B:673:ASN:H	1.86	0.41
1:A:126:PHE:CG	1:A:127:GLY:N	2.88	0.41
1:B:465:LEU:HB3	1:B:491:GLU:HB2	2.03	0.41
1:A:642:ALA:O	1:A:652:ASP:HB2	2.21	0.41
1:A:292:LYS:HB2	1:A:322:ASP:HB3	2.02	0.40
1:A:403:ASP:HB2	1:A:440:ARG:HG2	2.03	0.40
1:B:96:SER:C	1:B:97:ASP:OD1	2.64	0.40
1:B:203:LEU:HB3	1:B:211:ASP:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	649/723 (90%)	610 (94%)	32 (5%)	7 (1%)	11	26
1	B	658/723 (91%)	606 (92%)	40 (6%)	12 (2%)	6	15
All	All	1307/1446 (90%)	1216 (93%)	72 (6%)	19 (2%)	8	19

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	MET
1	B	75	ALA
1	B	78	SER
1	B	90	ARG
1	B	558	MET
1	A	421	GLU
1	A	623	GLU
1	B	76	GLN
1	A	67	ALA
1	B	97	ASP
1	B	555	ARG
1	A	246	PRO
1	B	177	ALA
1	B	624	GLY
1	A	248	ARG
1	A	420	ALA
1	B	192	GLY
1	B	89	PRO
1	B	479	SER

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	523/572 (91%)	492 (94%)	31 (6%)	18	38
1	B	527/572 (92%)	496 (94%)	31 (6%)	18	38
All	All	1050/1144 (92%)	988 (94%)	62 (6%)	18	38

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
1	A	69	SER
1	A	78	SER
1	A	82	ILE
1	A	97	ASP
1	A	134	THR
1	A	185	GLU
1	A	193	GLU
1	A	194	LEU
1	A	198	VAL
1	A	201	SER
1	A	228	THR
1	A	247	SER
1	A	248	ARG
1	A	309	LEU
1	A	313	GLU
1	A	332	THR
1	A	389	THR
1	A	415	LEU
1	A	479	SER
1	A	525	ASP
1	A	553	SER
1	A	566	THR
1	A	580	SER
1	A	592	SER
1	A	631	LEU
1	A	670	VAL
1	A	680	VAL
1	A	714	THR
1	A	717[A]	THR
1	A	717[B]	THR
1	B	76	GLN
1	B	90	ARG

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Mol	Chain	Res	Type
1	B	165	ILE
1	B	201	SER
1	B	256	VAL
1	B	267	LEU
1	B	305	VAL
1	B	307	ASP
1	B	312	VAL
1	B	313	GLU
1	B	332	THR
1	B	341	MET
1	B	444	LYS
1	B	448	MET
1	B	452	MET
1	B	460	THR
1	B	467	SER
1	B	509	SER
1	B	510	VAL
1	B	553	SER
1	B	558	MET
1	B	559	MET
1	B	562	SER
1	B	566	THR
1	B	620	THR
1	B	649	VAL
1	B	656	SER
1	B	689	THR
1	B	703	SER
1	B	717[A]	THR
1	B	717[B]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	304	ASN
1	A	315	GLN
1	A	507	ASN
1	A	531	ASN
1	A	536	GLN
1	A	547	GLN
1	B	253	ASN
1	B	665	ASN

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Mol	Chain	Res	Type
1	B	682	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	186:ARG	C	187:GLU	N	1.19

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	654/723 (90%)	0.21	17 (2%) 57 53	36, 61, 97, 127	1 (0%)
1	B	658/723 (91%)	0.57	48 (7%) 21 18	49, 73, 109, 135	2 (0%)
All	All	1312/1446 (90%)	0.39	65 (4%) 34 30	36, 67, 106, 135	3 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	66	LEU	5.9
1	B	559	MET	5.4
1	B	66	LEU	5.4
1	B	695	ALA	5.3
1	B	93	VAL	5.1
1	A	559	MET	5.1
1	B	558	MET	5.0
1	B	448	MET	4.9
1	A	446	GLY	4.6
1	B	445	SER	4.5
1	B	75	ALA	4.3
1	B	509	SER	4.3
1	B	94	PRO	4.2
1	B	78	SER	4.0
1	A	338	MET	3.6
1	A	449	GLY	3.5
1	B	74	VAL	3.5
1	B	388	MET	3.5
1	B	79	PRO	3.3
1	B	77	SER	3.3
1	B	194	LEU	3.3
1	B	447	HIS	3.2
1	A	444	LYS	3.1
1	B	338	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	387	MET	3.1
1	A	91	GLN	3.0
1	A	624	GLY	3.0
1	B	556	GLU	3.0
1	B	510	VAL	2.9
1	B	514	ASP	2.9
1	A	229	GLY	2.9
1	B	98	GLY	2.9
1	B	90	ARG	2.8
1	A	556	GLU	2.8
1	A	92	PRO	2.8
1	B	92	PRO	2.8
1	B	432	ASP	2.7
1	A	391	TYR	2.6
1	A	560	GLY	2.6
1	B	222	LEU	2.6
1	A	561	SER	2.5
1	B	698	ALA	2.5
1	B	76	GLN	2.4
1	B	723	PHE	2.4
1	B	97	ASP	2.4
1	B	391	TYR	2.3
1	B	672	ARG	2.3
1	B	668	TYR	2.3
1	A	571	ARG	2.3
1	B	130	LEU	2.2
1	B	147	MET	2.2
1	B	446	GLY	2.2
1	A	300	PHE	2.2
1	A	450	HIS	2.2
1	B	573	MET	2.2
1	B	282	ALA	2.1
1	B	584	THR	2.1
1	B	557	GLY	2.1
1	B	71	VAL	2.1
1	B	626	TRP	2.1
1	B	244	THR	2.0
1	B	449	GLY	2.0
1	B	530	TYR	2.0
1	B	138	MET	2.0
1	B	620	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AG	B	802	1/1	0.90	0.18	157,157,157,157	0
2	AG	A	801	1/1	0.93	0.08	91,91,91,91	0
2	AG	B	801	1/1	0.94	0.07	96,96,96,96	0
2	AG	A	802	1/1	0.94	0.15	136,136,136,136	0
2	AG	A	803	1/1	0.95	0.08	142,142,142,142	0
2	AG	B	803	1/1	0.97	0.05	124,124,124,124	0

6.5 Other polymers [i](#)

There are no such residues in this entry.